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Large-order shifted $1/N$ expansions through the asymptotic iteration method

T. Barakat *
Physics Department, King saud University,
Riyadh 11451, Saudi Arabia

Abstract

The perturbation technique within the framework of the asymptotic iteration method is used to obtain large-order shifted $1/N$ expansions, where N is the number of spatial dimensions. This method is contrary to the usual Rayleigh-Schrödinger perturbation theory, no matrix elements need to be calculated. The method is applied to the Schrödinger equation and the non-polynomial potential $V(r) = r^2 + \frac{br^2}{(1+cr^2)}$ in three dimensions is discussed as an illustrative example.

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*electronic address: tbarakat@ksu.edu.sa

1 Introduction

The shifted $1/N$ expansion technique (SLNT) proposed by Sukhatme and Imbo [1] is an extremely powerful method of solving Schrödinger equation, and has been used extensively to determine the eigenenergies for some important potentials [2-6]. The SLNT is an expansion in powers of $\Lambda^{-1/2}$, $\Lambda = N + 2\ell - a$, where N, ℓ and a stand for the number of dimensions, the angular momentum quantum number, and a is a properly chosen shift parameter, respectively. The shift parameter a is usually chosen so as to improve the convergence of the energy perturbation series, and to obtain the correct answer for the harmonic oscillator and the hydrogen atom to all orders.

After expanding the potential-energy function and the centrifugal term in Taylor series about an appropriate point r_0 one is left with the Hamiltonian operator for a harmonic oscillator plus a polynomial perturbation. Then one applies perturbation theory and obtains the perturbation corrections for the eigenfunctions and eigenenergies.

The Rayleigh-Schrödinger and the logarithmic perturbation schemes (referred to as RSPT and LPT respectively) have been used for the calculation of these corrections.

As well known the applications of the above two schemes were restricted by serious difficulties. They require considerable computational time and effort, and they involve, in general, quite elaborate algebraic manipulations, so it was extremely laborious to advance beyond the first four perturbation expansion terms in the eigenenergy series [2].

On the other hand, considerable progress was made in the last few years to obtain large-order shifted $1/N$ expansions [7-10]. For example, Maluendes et al. [7] reported an approach in which the coefficients of the SLNT of arbitrarily high orders could be generated by means of the hypervirial (HV) and Hellmann-Feynman theorems (HF), and thereby providing an excellent check for the convergence of the method.

However, the previous authors in their work did not give explicit expressions of their algorithm, each order getting progressively much more complicated than the previous one, and the derivations were tediously long. Thus, the need arises here to have a relatively simple, fast and effective method that provides large-order shifted $1/N$ expansions.

The so-called perturbation technique within the framework of the asymptotic iteration method (AIM) [11] have emerged in recent years to be a very useful and powerful technique of attack. This method reproduced excellent results for many important potentials in relativistic and non-relativistic quantum mechanics. Through AIM one can actually obtain all the perturbation corrections to both energy level shifts and wavefunctions for all states [12, 13]. These quantities can be calculated to any given accuracy, since the generation of successive corrections in the present perturbative framework, only requires the solution of simple algebraic equation.

The method is also applicable in the same form to both the ground state and excited bound states without involving tedious calculations which appeared in the available perturbation theories.

Encouraged by its satisfactory performance, we feel tempted to extend AIM, and to see this time how the AIM can be used to obtain large-order shifted $1/N$ expansions for the three-dimensional Schrödinger equation with any arbitrary spherically

symmetric potential $V(r)$ directly without either, using the base eigenfunctions of the unperturbed problem, or needing to calculate matrix elements.

As an illustration, the present technique is applied to the non-polynomial potential $V(r) = r^2 + \frac{br^2}{(1+cr^2)}$. This potential appears in several areas of physics. In field theory it provides a simple zero-dimensional model possessing a non-polynomial Lagrangian [14]. In laser physics it arises out of the Fokker-Planck equation for a single-mode laser [15].

For this potential only a class of exact analytical solutions for certain parameter dependence $b = b(c)$ were obtained [16, 17]. Hence, it has been a subject of several investigations and many authors have studied the one-, two-and three-dimensional cases [18, 19]. Roy, Roychoudhury and Roy have shown the supersymetric character of this potential and given new solutions using the standard $1/N$ expansion method [20].

With this in mind, this paper is organized as follows. In Sec. 2, the formulation of SLNT through AIM is outlined to find the eigenenergies for any arbitrary spherically symmetric potential. The analytical expressions for AIM are cast in such a way that allows the reader to use them without proceeding into their derivation. In Sec. 3, we explained how to obtain numerically the eigenenergies for the non-polynomial potential $V(r) = r^2 + \frac{br^2}{(1+cr^2)}$, and therein we will compare the accuracy of our results with those obtained by Roy et al. [20]. Finally, the paper ends with a brief summary and concluding remarks on the method and our findings.

2 Formalism of the asymptotic iteration method for SLNT

The radial part of the time-independent Schrödinger equation for central-field model in terms of the expansion parameter Λ in N- dimensional space with ($\hbar =$

$2m = 1$) is

$$\left\{-\frac{d^2}{dr^2} + \frac{\Lambda^2}{4r^2}(1 + \frac{2A}{\Lambda} + \frac{4B}{\Lambda^2})\right\}\chi_{n\ell}(r) = E_{n\ell}\chi_{n\ell}(r), \tag{1}$$

with

$\Lambda = N + 2\ell - a, \quad A = 1 - N + a, \quad B = (N - a)(N - a - 2)/4.$

SLNT begins with shifting the origin of the coordinate through the definition

$$x = \Lambda^{1/2}(\frac{r}{r_0} - 1), \tag{2}$$

where r_0 is chosen to minimize the effective potential $V_{eff}(r) = \Lambda^2(\frac{1}{4r^2} + \frac{V(r)}{\Lambda^2})$, so that

$$\Lambda^2 = 2r_0^3 V'(r_0). \tag{3}$$

Expansions about $r = r_0$, yield

$$\left\{-\frac{d^2}{dx^2} + \sum_{i=0}^{\infty}(\alpha_i g^i x^{i+2} + \beta_i g^i x^i + \xi_i g^{i+2} x^i)\right\}\chi_{n\ell}(x) = \epsilon_{n\ell}\chi_{n\ell}(x) \tag{4}$$

where

$$\alpha_i = (-1)^i\frac{i+3}{4} + \frac{r_0^{i+1}}{2(i+2)!}\frac{d^{i+2}V(r_0)}{V'(r_0)dr_0^{i+2}}, \ \beta_i = (-1)^i\frac{i+1}{2}A, \ \xi_i = (-1)^i(i+1)B, \tag{5}$$

and

$$\epsilon_{n\ell} = r_0^2 g^2(E_{n\ell} - V_{eff}(r_0)), \text{ and } \ g = 1/\Lambda^{1/2}. \tag{6}$$

The systematic procedure of the AIM begins now by expanding the eigenenergy

term in powers of g, and rewriting equation (4) in the following form

$$\left[-\frac{d^2}{dx^2}+\alpha_0x^2+\beta_0+g(\alpha_1x^3+\beta_1x)+g^2(\alpha_2x^4+\beta_2x^2+\xi_0)\right.$$

$$\left.+g^3(\alpha_3x^5+\beta_3x^3+\xi_1x)+g^4(\alpha_4x^6+\beta_4x^4+\xi_2x^2)+\cdots\right]\chi_{n\ell}(r)$$

$$=\left[\epsilon^{(0)}_{n\ell}+g\epsilon^{(1)}_{n\ell}+g^2\epsilon^{(2)}_{n\ell}+g^3\epsilon^{(3)}_{n\ell}+g^4\epsilon^{(4)}_{n\ell}+\cdots\right]\chi_{n\ell}(x). \tag{7}$$

If we further insert the ansatz

$$\chi_{n\ell}(x)=e^{-\gamma x^2/2}f_{n\ell}(x) \tag{8}$$

into equation (7), carrying out the mathematics, in this case, the function $f_{n\ell}(x)$ will satisfy a new second-order homogeneous linear differential equation of the form

$$f^{''}_{n\ell}(x)=\lambda_0(x,g)f^{'}_{n\ell}(x)+s_0(x,g)f_{n\ell}(x), \tag{9}$$

where $\lambda_0(x,g)=2\gamma x$, and

$$\begin{aligned} s_0(x,g) &= (\alpha_0-\gamma^2)x^2+\beta_0+\gamma-\epsilon_{n\ell}+g(\alpha_1x^3+\beta_1x)+g^2(\alpha_2x^4+\beta_2x^2+\xi_0) \\ &+ g^3(\alpha_3x^5+\beta_3x^3+\xi_1x)+g^4(\alpha_4x^6+\beta_4x^4+\xi_2x^2)+\cdots, \end{aligned} \tag{10}$$

$$\epsilon_{n\ell}=\epsilon^{(0)}_{n\ell}+g\epsilon^{(1)}_{n\ell}+g^2\epsilon^{(2)}_{n\ell}+g^3\epsilon^{(3)}_{n\ell}+g^4\epsilon^{(4)}_{n\ell}+..... \tag{11}$$

Here, it should be pointed out that, the choice of g in equation (9) will be motivated, that is when we switch off g, equation (9) will be reduced to an exactly solvable eigenvalue problem within the framework of AIM [21-23].

To apply the perturbation expansion technique within the framework of AIM we rely on the symmetric structure of the right hand side of equation (9). Thus, we

differentiate equation (9) $(k+2)$ times with respect to x, $k = 1, 2, ...$ Then we take the ratio of the $(k+2)^{th}$ and $(k+1)^{th}$ derivatives, and for sufficiently large k we introduce, respectively, the "asymptotic" aspect and the termination condition of the method, which, in turn will lead to

$$\varrho(x,g) \equiv \frac{s_k(x,g)}{\lambda_k(x,g)} = \frac{s_{k-1}(x,g)}{\lambda_{k-1}(x,g)}, \tag{12}$$

$$\delta_k(x,g) \equiv s_k(x,g)\lambda_{k+1}(x,g) - s_{k+1}(x,g)\lambda_k(x,g) = 0. \tag{13}$$

We now proceed to obtain the eigenenergies of equation (9) systematically in terms of the expansion parameter g. If we expand $\delta_k(x,g)$ around $g = 0$, we get the following series

$$\delta_k(x,g) = \delta_k(x,0) + \frac{g}{1!}\frac{\partial\delta_k(x,g)}{\partial g}|_{g=0} + \frac{g^2}{2!}\frac{\partial^2\delta_k(x,g)}{\partial g^2}|_{g=0} + \frac{g^3}{3!}\frac{\partial^3\delta_k(x,g)}{\partial g^3}|_{g=0} + ...(14)$$

According to the procedure of AIM [21-23], $\delta_k(x,g)$ must be zero; if this to be true for every g value, then every term of the series must be zero. That is to say

$$\delta_k^{(j)}(x,g) = \frac{g^j}{j!}\frac{\partial^j\delta_k(x,g)}{\partial g^j}|_{g=0} = 0, \quad j = 0, 1, 2.... \tag{15}$$

A quantitative estimate for $\epsilon_{n\ell}$ expansion terms can be obtained by comparing the terms with the same order of g in equations (9) and (14). Therefore, it is clear that the roots of $\delta_k^{(0)}(x,0) = 0$ give us the zero'th contribution energy terms $\epsilon_{n\ell}^{(0)}$. Likewise, the roots of $\delta_k^{(1)}(x,g)|_{g=0} = 0$ give us the first correction terms $\epsilon_{n\ell}^{(1)}$, and so on. Therefore, the general solution for the eigenenergies $E_{n\ell}$ in conjunction with equations (6) and (11) is

$$E_{n\ell} = \frac{\Lambda^2}{r_0^2}\left(\frac{1}{4} + \frac{r_0^2 V(r_0)}{\Lambda^2}\right) + \frac{1}{r_0^2 g^2}\sum_{i=0}^{\infty} g^i \epsilon_{n\ell}^{(i)}. \tag{16}$$

3 Numerical results for the eigenenergies of the potential $V(r) = r^2 + \frac{br^2}{(1+cr^2)}$

Within the framework of the asymptotic iteration method mentioned in the above section, the eigenenergies $E_{n\ell}$ of the non-polynomial potential $V(r) = r^2 + \frac{br^2}{(1+cr^2)}$ are calculated by means of equation (16).

To obtain the zero'th contribution energy terms $\epsilon^{(0)}_{n\ell}$, one should simply switch off g in equation (9), that will lead to an exactly solvable eigenvalue problem within the framework of AIM,

$$f^{''}_{n\ell}(x) = 2\gamma x f^{'}_{n\ell}(x) + \left((\alpha_0 - \gamma^2)x^2 + \beta_0 + \gamma - \epsilon^{(0)}_{n\ell}\right) f_{n\ell}(x). \tag{17}$$

For each iteration, the expression $\delta^{(0)}_k(x,0) = 0$ in equation (13) depends on two variables namely γ and x. Since the problem is exactly solvable, the calculated eigenenergies $\epsilon^{(0)}_{n\ell}$ by means of this condition are independent of the choice of x once we set $\gamma = \sqrt{\alpha_0}$; then the roots of $\delta^{(0)}_k(x,0) = 0$ are

$$\epsilon^{(0)}_{n\ell} = \beta_0 + (2n+1)(\alpha_0)^{1/2}, \qquad n = 0, 1, 2, ... \tag{18}$$

As we noted before, the leading contribution term of the total energy is of order Λ^2 given in equation (16). The next contribution is of order Λ and is given by $\beta_0 + (2n+1)(\alpha_0)^{1/2}$. It is customary to choose the shift parameter a so as to make this contribution vanish. This choice is physically motivated by requiring agreement between the $1/\Lambda$ expansions and the exact analytic results for the harmonic-oscillator and Coulomb potentials to all orders [2]. However, there are some difficult cases in which this simple choice is insufficient and it is really necessary to select an order-dependent value of a according to minimal sensitivity or other appropriate criterion [7]. Nevertheless, at this point, it is enough for us to compare the AIM results with

the SLNT results. Therefore, we choose

$$a = 2 - 2(2n+1)(\alpha_0)^{1/2}, \tag{19}$$

$\Lambda = N + 2\ell - a$, and $\Lambda^2 = 2r_0^3 V'(r_0)$. Collecting these terms and carrying out the mathematics, one can get

$$3 + 2\ell - 2 + 2(2n+1)(\alpha_0)^{1/2} = (2r_0^3 V'(r_0))^{1/2}, \tag{20}$$

which is an implicit equation for r_0. Once r_0 is determined, the leading term $\Lambda^2 V_{eff}(r_0)$ can be calculated numerically. On the other hand, to obtain the higher order perturbative expansion terms, first one should go to equation (9) switch on g and then replace $\epsilon_{n\ell}$ with $\epsilon_{n\ell}^{(0)} + g\epsilon_{n\ell}^{(1)}$, and terminate the iterations by imposing the condition $\delta_k^{(1)}(x, g) = 0$ as an approximation to equation (9). The first root of the resulting equation gives $\epsilon_{n\ell}^{(1)}$. Similarly, and very easily one can obtain the other perturbative expansion terms.

Throughout the present calculations, it is observed that the perturbation corrections of odd orders $\epsilon_{n\ell}^{(2i+1)}$ are vanish for all i.

In table 1 an explicit list of calculations up to six'th order with different values of ℓ, b, and c are given, so that the reader may, if so inclined, reproduce our results. In table 2 the results of AIM, together with the standard shifted expansion method $E_{n\ell}(1/N)$ and the exact super-symmetric results are displayed for comparison purposes.

In tables we have only considered the eigenenergies for the ground state $n = 0$. This was in order to make a clear comparison between the results of this method and the results of [20]. Examination of tables shows that the accuracy of the AIM is better than the accuracy of shifted 1/N expansion method, and the predicted

eigenenergies $E_{n\ell}$(AIM) are all in excellent agreement with the results of the supersymmetric method [20].

We have also shown that, it is very easy task to implement the perturbation technique within the framework of the AIM without having to be worry about the ranges of the couplings in the potential.

This method is also applicable in the same form to both the ground state, and excited bound states without involving tedious calculations which appeared in the available perturbation theories.

As a concluding remark, the present method enable one if it is necessary, to keep a as a free parameter up to the end of the calculations. With this choice the results can be drastically improved by raising up the perturbative order in the expansion to any order, and then one can determine the value of a according to the minimal sensitivity method or any other appropriate criterion.

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Table 1: The calculated values of the coefficients in the energy expansion $\epsilon_{n\ell}$ for the non-polynomial potential by means of this work with different values of ℓ, b, and c.

ℓ	c	b	$\epsilon_{0\ell}^{(0)}$	$\epsilon_{0\ell}^{(1)}$	$\epsilon_{0\ell}^{(2)}$	$\epsilon_{0\ell}^{(3)}$	$\epsilon_{0\ell}^{(4)}$	$\epsilon_{0\ell}^{(5)}$	$\epsilon_{0\ell}^{(6)}$
0	0.1	-0.46	0	0	-0.021504914	0	0.01472806	0	-0.010867
1	0.1	-0.5	0	0	-0.030894587	0	0.02042523	0	-0.0034827
2	0.1	-0.54	0	0	-0.034627947	0	0.01793987	0	0.018511
0	0.01	-0.0406	0	0	-0.000018842	0	1.707706x10^{-}6	0	-1.7717x10^{-}6
1	0.01	-0.041	0	0	-0.000049912	0	7.312060x10^{-}6	0	-7.6296x10^{-}6
-1	0.1	-0.42	0	0	-0.005539564	0	0.002341067	0	-0.0018839

Table 2: Comparison between selected eigenenergies calculated from the standard shifted (1/N) expansion method $E_{n\ell}(1/N)$ [20], the exact super-symmetric values $E_{n\ell}(SUSY)$ [20], and the eigenenergies $E_{n\ell}(AIM)$ computed by means of equation (16) up to four'th and six'th orders.

ℓ	c	b	$E_{0\ell}(1/N)$	$E_{0\ell}(SUSY)$	$E_{0\ell}^{4th}(AIM)$	$E_{0\ell}^{6th}(AIM)$
0	0.1	-0.46	2.400520	2.4	2.40051591814138	2.3999024133815471
1	0.1	-0.5	4.000116	4.0	4.00012195111641	4.0000777082899992
2	0.1	-0.54	5.599965	5.6	5.59998537049538	5.6000735787721094
0	0.01	-0.0406	2.939999	2.94	2.94000001431155	2.9399998857627638
1	0.01	-0.041	4.899974	4.9	4.90000002136554	4.8999999017683162
-1	0.1	-0.041	0.801177	0.8	0.80117658318143	0.7984848338375296